ethyl 2-acetyloxypropanoate

2985-28-6 | DTXSID00277952

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.87	0.81	0.87	0.82	0.86	0.86

Model Results

Predicted value: 2.26e-01 mol/L

Global applicability domain: Inside

Local applicability domain index: 8.84e-01

Confidence level: 7.11e-01

Nearest Neighbors from the Training Set

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ethyl 2-acetyloxypropanoate
Measured: 2.00e-01
Predicted: 2.26e-01

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Propanoic acid, 2-(1-oxopropoxy)-, methyl ester
Measured: 1.37e-01
Predicted: 2.58e-01

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Propylene glycol diacetate
Measured: 6.24e-01
Predicted: 3.94e-01

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1,3-Propanediol, diacetate
Measured: 6.24e-01
Predicted: 4.12e-01

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2-Propene-1,1-diol diacetate
Measured: 5.69e-02
Predicted: 1.05e-01